

Hexachlorophene
70-30-4 | DTXSID6020690

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 4670

Global applicability domain: Inside

Local applicability domain index: 3.35e-01

Confidence level: 6.93e-01

Nearest Neighbors from the Training Set

Image not found

Bromofos

Measured: 3890

Predicted: 1330

Image not found

Fenchlorphos

Measured: 3800

Predicted: 597

Image not found

2,2,4,5,6,7,8-Octachloro-
2,3,3a,4,7,7a-hexahydro-4,7-
methano-1H-indene

Measured: 20000

Predicted: 15100

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Iodenphos

Measured: 4170

Predicted: 1220